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L2 2 SEA SSS SAM L1

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FULL SCREEN SEARCH COMPLETED - 159 TO ITERATE

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ENTRY SESSION
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L4 10 L3

=> d 14 1- ibib abs hitstr

YOU HAVE REQUESTED DATA FROM 10 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2000 ACS ACCESSION NUMBER: 1999:764041 CAPLUS

DOCUMENT NUMBER: 132:22971

TITLE: Preparation of oxopyrido- and -pyrimidopyrimidines as

cellular proliferation inhibitors

INVENTOR(S): Dobrusin, Ellen Myra; Hamby, James Marino; Kramer,

James Bernard; Schroeder, Mel Conrad; Showalter,

Howard Daniel Hollis; Toogood, Peter;

Trumpp-Kallmeyer, Susanne A.

PATENT ASSIGNEE(S): Warner-Lambert Co., USA

SOURCE: PCT Int. Appl., 133 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. KI | | | | ND | DATE | | | A | PPLI | CATI | ои и | o. : | DATE | | | | |
|---|---------|-----|-----|------------------|------|-----|--------------------------|-----|------|------|-------|------|------|------|------|-----|-----|
| | | | | | | | | | _ | | | | | | | | |
| WO | 9961444 | | A | A2 19991202 | | | WO 1999-US10187 19990510 | | | | | | | | | | |
| | W: | ΑE, | AL, | ΑU, | BA, | BB, | BG, | BR, | CA, | CN, | CU, | CZ, | EE, | GD, | GE, | HR, | HU, |
| | | ID, | IL, | IS, | JP, | ΚP, | KR, | LC, | LK, | LR, | LT, | LV, | MG, | MK, | MN, | MX, | NO, |
| | | ΝZ, | PL, | RO, | SG, | SI, | SK, | SL, | TR, | TT, | UA, | US, | UΖ, | VN, | YU, | ZA, | AM, |
| | | ΑZ, | BY, | KG, | ΚZ, | MD, | RU, | ТJ, | TM | | | | | | | | |
| | RW: | GH, | GM, | ΚE, | LS, | MW, | SD, | SL, | SZ, | UG, | ZW, | ΑT, | ΒÉ, | CH, | CY, | DE, | DK, |
| | | ES, | FI, | FR, | GB, | GR, | ΙE, | ΙT, | LU, | MC, | NL, | PT, | SE, | BF, | ВJ, | CF, | CG, |
| | | CI, | CM, | GΑ, | GN, | GW, | ML, | MR, | NE, | SN, | TD, | TG | | | | | |
| PRIORITY APPLN. INFO.: US 1998-86708 19980526 | | | | | | | | | | | | | | | | | |
| | | | | | | | | | U | S 19 | 99-1: | 2615 | 8 | 1999 | 0325 | | |
| OTHER SOURCE(S): | | | | MARPAT 132:22971 | | | | | | | | | | | | | |

GΙ

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R8 R9 R4 R3
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INDEX NAME)

AB Title compds. [I; G = NR2 or CHR2; R = NHR1 or SO0-2R1; R1, R2 = H, (cyclo)alkyl, (un)substituted PH, -pyridyl, etc.; R3 = groups cited for R1, OH, alkoxy(carbonyl), etc.; R4 = H; R3R4 = bond; R8,R9 = H, halo, NH2, alkoxycarbonyl, etc.; X = O, S, (alkyl)imino, etc.; Z =N or CH] were prepd. as cyclin-dependant and tyrosine kinase inhibitors. Thus, 5-aminomethyl-4-cyclopentylamino-2-methylthiopyrimidine (prepn. given) was cyclocondensed with 1,1'-carbonyldiimidazole and the oxidized product aminated by 4-(MeO) C6H4NH2 to give I [G = cyclopentylimino, R = 4-(MeO)C6H4NH, R3 = R4 = R8 = R9 = H, X = O]. Data for biol. activity of I were given. TT 251370-13-5P 251370-14-6P 251370-15-7P 251370-16-8P 251370-17-9P 251370-18-0P 251370-19-1P 251370-20-4P 251370-21-5P 251370-22-6P 251370-23-7P 251370-24-8P 251370-25-9P 251370-26-0P 251370-27-1P 251370-28-2P 251370-29-3P 251370-30-6P 251370-31-7P 251370-32-8P 251370-33-9P 251370-66-8P 251370-67-9P 251370-68-0P 251371-07-0P 251371-08-1P 251371-09-2P 251371-10-5P 251371-11-6P 251371-12-7P 251371-13-8P 251371-14-9P 251371-17-2P 251371-18-3P 251371-19-4P 251371-20-7P 251371-21-8P 251371-22-9P 251371-89-8P 251371-90-1P 251371-91-2P 251371-92-3P 251371-93-4P RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of bicyclic pyrimidines and bicyclic 3,4-dihydropyrimidines as inhibitors of cellular proliferation) RN 251370-13-5 CAPLUS CN Piperazine, 1-(aminoacetyl)-4-[4-[6-(3,5-dimethoxyphenyl)-8-ethyl-5,6,7,8-

tetrahydro-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]phenyl]- (9CI) (CA

Page 4

$$\begin{array}{c|c} O \\ \hline \\ C - CH_2 - NH_2 \\ \hline \\ MeO \end{array}$$

RN 251370-14-6 CAPLUS

CN Piperazine, 1-(aminoacetyl)-4-[4-[[6-(2-chloro-3,5-dimethoxyphenyl)-8-

ethyl-5,6,7,8-tetrahydro-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 251370-15-7 CAPLUS

CN Piperazine,

1-(aminoacetyl)-4-[4-[[6-(2,6-dichloro-3,5-dimethoxyphenyl)-8-

ethyl-5,6,7,8-tetrahydro-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]phenyl](9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN 251370-16-8 CAPLUS

CN Piperazine, 1-(aminoacetyl)-4-[4-[[6-(3,5-dimethoxy-2-methylphenyl)-8-

ethyl-5,6,7,8-tetrahydro-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

RN 251370-17-9 CAPLUS

CN Piperazine,

1-(aminoacetyl)-4-[4-[6-(3,5-dimethoxy-2,6-dimethylphenyl)-8-

ethyl-5,6,7,8-tetrahydro-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

RN 251370-18-0 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one,

7-[[4-[2-(diethylamino)ethoxy]phenyl]a

mino]-3-(3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro- (9CI) (CA INDEX NAME)

RN 251370-19-1 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one,

3-(2-chloro-3,5-dimethoxyphenyl)-7-[[4-

[2-(diethylamino)ethoxy]phenyl]amino]-1-ethyl-3,4-dihydro- (9CI) (CA INDEX NAME)

RN 251370-20-4 CAPLUS

CN Pyrimido [4,5-d] pyrimidin-2(1H)-one,

3-(2,6-dichloro-3,5-dimethoxyphenyl)-7-

[[4-[2-(diethylamino)ethoxy]phenyl]amino]-1-ethyl-3,4-dihydro- (9CI) (CA INDEX NAME)

RN 251370-21-5 CAPLUS
CN Pyrimido[4,5-d]pyrimidin-2(1H)-one,
7-[[4-[2-(diethylamino)ethoxy]phenyl]a
 mino]-3-(3,5-dimethoxy-2-methylphenyl)-1-ethyl-3,4-dihydro- (9CI) (CA INDEX NAME)

RN 251370-22-6 CAPLUS
CN Pyrimido[4,5-d]pyrimidin-2(1H)-one,
7-[[4-[2-(diethylamino)ethoxy]phenyl]a
 mino]-3-(3,5-dimethoxy-2,6-dimethylphenyl)-1-ethyl-3,4-dihydro- (9CI)
(CA
 INDEX NAME)

RN 251370-23-7 CAPLUS
CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 7-[[4-(diethylamino)butyl]amino]-3-(3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Et} & \text{OMe} \\ \text{Et}_2\text{N} - (\text{CH}_2)_4 - \text{NH} & \text{N} & \text{N} \end{array}$$

RN 251370-24-8 CAPLUS CN Pyrimido[4,5-d]pyrimidin-2

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(2-chloro-3,5-dimethoxyphenyl)-7-[[4-

(diethylamino)butyl]amino]-1-ethyl-3,4-dihydro- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Et}_{2}\text{N-} \left(\text{CH}_{2}\right)_{4} - \text{NH} & \\ \text{N} & \\ \text{N} & \\ \text{N} & \\ \text{OMe} & \\ \end{array}$$

RN 251370-25-9 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one,

3-(2,6-dichloro-3,5-dimethoxyphenyl)-7-

[[4-(diethylamino)butyl]amino]-1-ethyl-3,4-dihydro- (9CI) (CA INDEX NAME)

RN 251370-26-0 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 7-[[4-(diethylamino)butyl]amino]-3-(3,5-dimethoxy-2-methylphenyl)-1-ethyl-3,4-dihydro-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Et}_{2N^{-}} \text{ (CH}_{2}) \text{ 4-NH} & \text{N} & \text{O} \\ & & & \text{N} & \text{N} & \text{O} \\ & & & \text{N} & \text{OMe} \end{array}$$

RN 251370-27-1 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 7-[[4-(diethylamino)butyl]amino]-3-(3,5-dimethoxy-2,6-dimethylphenyl)-1-ethyl-3,4-dihydro-(9CI) (CA INDEX NAME)

Et₂N- (CH₂)
$$4$$
-NH N N O Me OMe OMe

RN 251370-28-2 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro-7-(4-pyridinylamino)- (9CI) (CA INDEX NAME)

RN 251370-29-3 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(2-chloro-3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro-7-(4-pyridinylamino)- (9CI) (CA INDEX NAME)

RN 251370-30-6 CAPLUS
CN Pyrimido[4,5-d]pyrimidin-2(1H)-one,
3-(2,6-dichloro-3,5-dimethoxyphenyl)-1ethyl-3,4-dihydro-7-(4-pyridinylamino)- (9CI) (CA INDEX NAME)

RN 251370-31-7 CAPLUS
CN Pyrimido[4,5-d]pyrimidin-2(1H)-one,
3-(3,5-dimethoxy-2,6-dimethylphenyl)-1 ethyl-3,4-dihydro-7-(4-pyridinylamino)- (9CI) (CA INDEX NAME)

RN 251370-32-8 CAPLUS
CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(3,5-dimethoxy-2-methylphenyl)-1-ethyl-3,4-dihydro-7-(4-pyridinylamino)- (9CI) (CA INDEX NAME)

RN 251370-33-9 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 1-cyclopentyl-3-(2,6-dichloro-3,5-dimethoxyphenyl)-3,4-dihydro-7-(4-pyridinylamino)- (9CI) (CA INDEX NAME)

RN 251370-66-8 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-[[4-(diethylamino)butyl]amino]-3-(3,5-dimethoxyphenyl)-1-ethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Et}_2\text{N}-\text{(CH}_2)\text{ 4-NH} & \text{N} & \text{OMe} \\ \hline \\ \text{N} & \text{N} & \text{OMe} \end{array}$$

RN 251370-67-9 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-[[4-[2-(diethylamino)ethoxy]phenyl]amino]-3-(3,5-dimethoxyphenyl)-1-ethyl- (9CI) (CA INDEX NAME)

RN 251370-68-0 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 3-(3,5-dimethoxyphenyl)-1-ethyl-7-(4-pyridinylamino)- (9CI) (CA INDEX NAME)

RN 251371-07-0 CAPLUS

CN Benzoic acid, 3-[[6-(2,6-dichlorophenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]- (9CI) (CA INDEX NAME)

RN 251371-08-1 CAPLUS

CN Benzamide, 3-[[6-(2,6-dichlorophenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]-N-[3-(dimethylamino)propyl]-(9CI)

(CA INDEX NAME)

RN 251371-09-2 CAPLUS

CN Benzamide, 3-[[6-(2,6-dichloro-3-hydroxyphenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]-N-[3-(dimethylamino)propyl]- (9CI) (CA INDEX NAME)

RN 251371-10-5 CAPLUS

CN Benzoic acid, 3-[[6-(2,6-dichloro-3-hydroxyphenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]- (9CI) (CA INDEX NAME)

RN 251371-11-6 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(2,6-dichlorophenyl)-7-[[4-[2-(ethylamino)ethoxy]phenyl]amino]-3,4-dihydro-1-methyl-(9CI) (CA INDEX NAME)

RN 251371-12-7 CAPLUS
CN Pyrimido[4,5-d]pyrimidin-2(1H)-one,
3-(2,6-dichloro-3-hydroxyphenyl)-7-[[4[2-(ethylamino)ethoxy]phenyl]amino]-3,4-dihydro-1-methyl- (9CI) (CA
INDEX
NAME)

RN 251371-13-8 CAPLUS
CN Benzamide, 4-[[6-(2,6-dichlorophenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & Me \\ H_2N-C & Me \\ \hline NH & N & O & C1 \\ \hline \end{array}$$

RN 251371-14-9 CAPLUS
CN Benzamide, 4-[[6-(2,6-dichloro-3-hydroxyphenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]- (9CI) (CA INDEX NAME)

RN 251371-17-2 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(2,6-dichloro-3-hydroxyphenyl)-3,4-dihydro-1-methyl-7-[[4-(4-morpholinyl)phenyl]amino]- (9CI) (CA INDEX NAME)

RN 251371-18-3 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(2,6-dichloro-3-hydroxyphenyl)-3,4-dihydro-7-[[3-(hydroxymethyl)phenyl]amino]-1-methyl- (9CI) (CA INDEX NAME)

RN 251371-19-4 CAPLUS

CN Benzenebutanoic acid, 4-[[6-(2,6-dichlorophenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]- (9CI) (CA INDEX NAME)

RN 251371-20-7 CAPLUS

CN Benzenebutanoic acid, 4-[[6-(2,6-dichloro-3-hydroxyphenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]- (9CI) (CA INDEX NAME)

$$Me$$

$$NH \qquad N \qquad N \qquad N \qquad O \qquad C1$$

$$NH \qquad N \qquad N \qquad N \qquad O \qquad C1$$

$$OH \qquad OH$$

RN 251371-21-8 CAPLUS

CN Benzaldehyde, 4-[[6-(2,6-dichlorophenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]- (9CI) (CA INDEX NAME)

RN 251371-22-9 CAPLUS

CN Benzaldehyde, 4-[[6-(2,6-dichloro-3-hydroxyphenyl)-5,6,7,8-tetrahydro-8-methyl-7-oxopyrimido[4,5-d]pyrimidin-2-yl]amino]- (9CI) (CA INDEX NAME)

RN 251371-89-8 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro-7-[[2-[(4-pyridinylmethyl)amino]ethyl]amino]- (9CI) (CA INDEX NAME)

RN 251371-90-1 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro-7-[[3-(4-methyl-1-piperazinyl)propyl]amino]- (9CI) (CA INDEX NAME)

RN 251371-91-2 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro-7-[[4-(4-methyl-1-piperazinyl)butyl]amino]- (9CI) (CA INDEX NAME)

Me N— (CH₂)
$$_4$$
 – NH N N OMe OMe

RN 251371-92-3 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 3-(3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro-7-[[5-(4-methyl-1-piperazinyl)pentyl]amino]- (9CI) (CA INDEX NAME)

RN 251371-93-4 CAPLUS

CN Pyrimido[4,5-d]pyrimidin-2(1H)-one, 7-[[3-(diethylamino)propyl]amino]-3-(3,5-dimethoxyphenyl)-1-ethyl-3,4-dihydro-(9CI) (CA INDEX NAME)

IT 251372-02-8P 251372-03-9P 251372-04-0P 251372-05-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of bicyclic pyrimidines and bicyclic 3,4-dihydropyrimidines as inhibitors of cellular proliferation)

RN 251372-02-8 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 1-(1-methylethyl)-7-[[4-(4-methyl-1-piperazinyl)phenyl]amino]-3-(2-propenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

$$\begin{array}{c|c} \text{i-Pr} & \text{O-CH}_2\text{-CH}_2\text{-NEt}_2\\ \text{O} & \text{N} & \text{NH} \\ \text{H}_2\text{C} = \text{CH-CH}_2 & \text{O} \end{array}$$

ANSWER 2 OF 10 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER:

1995:334056 CAPLUS

DOCUMENT NUMBER:

122:239631

TITLE:

Purines, pyrimidines and condensed systems based on them. 12. 1,3-Dimethylpyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione: the first case of regioselective amination of condensed pyrimidines at position 2 Gulevskaya, A. V.; Pozharsky, A. F.; Shorshnev, S.

AUTHOR (S): V.;

Zheltushkina, E. A.

CORPORATE SOURCE:

SOURCE:

Rostov. Gos. Univ., Rostov-on-Don, 344006, Russia Khim. Geterotsikl. Soedin. (1994), (9), 1249-52

CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

Amination of the title compd. in the presence of an oxidizing agent gave AΒ 7-amino derivs. (I; NR1R2 = NH2, NHMe, NHEt, NHCMe3, piperidino, morpholino); in the case of Me2NH the 4-substituted deriv. (II) was also formed. Successive hydrolysis of I (NR1R2 = piperidino) in alk. and acidic medium gave 4-(methylamino)-2-piperidinopyrimidine (III).

94839-44-8P 94839-45-9P 162147-58-2P IT

162147-59-3P RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of) 94839-44-8 CAPLUS RN

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-amino-1,3-dimethyl- (9CI) (CA INDEX NAME)

RN 94839-45-9 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 1,3-dimethyl-7-(methylamino)-(9CI) (CA INDEX NAME)

RN 162147-58-2 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-(ethylamino)-1,3-dimethyl-(9CI) (CA INDEX NAME)

RN 162147-59-3 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-[(1,1-dimethylethyl)amino]-1,3-dimethyl- (9CI) (CA INDEX NAME)

CAPLUS COPYRIGHT 2000 ACS ANSWER 3 OF 10

1994:134411 CAPLUS ACCESSION NUMBER:

120:134411

DOCUMENT NUMBER: TITLE:

Reactions of uracils. 21. Zwitterionic

heteropolycyclic uracils by a novel three-component reaction: iminophosphorane, isocyanate, heteroarene Wamhoff, Heinrich; Schmidt, Andreas

AUTHOR (S):

CORPORATE SOURCE:

Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, D-53121,

Germany

SOURCE:

J. Org. Chem. (1993), 58(25), 6976-84

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 120:134411

GΙ

The novel three-component reaction of (uracil-6-ylimino)phosphorane I, AΒ isocyanate, and (substituted) pyridines gives, in a one-pot procedure, a variety of new pyrido[1',2':3,4]pyrimido[4,5-d]pyrimidines, e.g., II (R = aryl, Me2CH, tosyl, allyl). The zwitterionic ground state of these new ring systems is established by solvatochromism, Hammett correlations,

NMR,

and X-ray anal. Replacement of the pyridine by isoquinoline and

09/ 422,451

phthalazine gives access to the novel ring systems pyrimido[4',5':4,5]pyrimido[6,1-a]isoquinoline and -phthalazine, which

are

formed as dihydro derivs. [III; X = CH, N (15); R = aryl] or as zwitterions, depending on the reaction conditions. Oxidative cleavage of the phthalazine 15 in nitrobenzene affords the (cyanophenyl)pyrimido[4,5-d]pyrimidines.

IT 152897-89-7P 152897-90-0P 152897-91-1P 152897-92-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and oxidn. or thermal cleavage of)

RN 152897-89-7 CAPLUS

CN Benzonitrile, 2-[5,6,7,8-tetrahydro-6,8-dimethyl-5,7-dioxo-2-(phenylamino)pyrimido[4,5-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

RN 152897-90-0 CAPLUS

CN Benzonitrile,

2-[2-[(4-chlorophenyl)amino]-5,6,7,8-tetrahydro-6,8-dimethyl-5,7-dioxopyrimido[4,5-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

RN 152897-91-1 CAPLUS

CN Benzonitrile, 2-[5,6,7,8-tetrahydro-6,8-dimethyl-5,7-dioxo-2-[[3-(trifluoromethyl)phenyl]amino]pyrimido[4,5-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

RN 152897-92-2 CAPLUS

CN Benzonitrile,

2-[5,6,7,8-tetrahydro-6,8-dimethyl-2-[(4-methylphenyl)amino]-5,7-dioxopyrimido[4,5-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2000 ACS ACCESSION NUMBER: 1992:531144 CAPLUS

DOCUMENT NUMBER: 117:131144

Cyclization reactions of chloro-substituted TITLE:

2-azoniaallene salts with bifunctional nucleophiles

AUTHOR(S): Hamed, Atef

Fac. Sci., Menoufia Univ., Shebin El-Koom, Egypt CORPORATE SOURCE:

SOURCE: Synthesis (1992), (6), 591-5

CODEN: SYNTBF; ISSN: 0039-7881

DOCUMENT TYPE: Journal

LANGUAGE: English GI

AB Multifunctional electrophilic chloro-substituted 2-azoniaallene salts react with bifunctional nucleophiles to furnish heterocycles. Thus, PhCCl:N+:CClPh SbCl6- reacts with pyrimidinedione I to give pyrimidopyrimidinedione salt II. Pyrimido-1,3-oxazin-1-ium salts, e.g., III, representing a new ring system, triazinium salts, e.g., IV, and a triazolium salt (V) are also obtained.

IT 143249-47-2P

RN 143249-47-2 CAPLUS

CN Antimonate(1-), hexachloro-, (OC-6-11)-, hydrogen, compd. with 7-(dimethylamino)-1,3-dimethylpyrimido[4,5-d]pyrimidine-2,4,5(1H,3H,6H)-trione (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 143249-46-1 CMF C10 H13 N5 O3

$$\begin{array}{c|c} & \text{Me} \\ \text{Me}_2 \text{N} & \text{H} & \text{N} \\ \text{N} & \text{N} & \text{N} \\ \text{N} & \text{N} & \text{Me} \\ \end{array}$$

CM 2

CRN 16941-91-6 CMF Cl6 Sb . H CCI CCS

CDES 7:0C-6-11

c1c1-

• H+

L4 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2000 ACS ACCESSION NUMBER: 1990:514913 CAPLUS

DOCUMENT NUMBER: 113:114913

TITLE: Pyrimidines. 63. Novel ring transformations of

5-cyanouracils into 2-thiocytosines,

2,4-diaminopyrimidines, and

pyrimido[4,5-d]pyrimidines

by the reaction with thioureas and guanidines

AUTHOR(S): Hirota, Kosaku; Sajiki, Hironao; Kitade, Yukio; Maki,

Yoshifumi

CORPORATE SOURCE: Gifu Pharm. Univ., Gifu, 502, Japan

SOURCE: J. Chem. Soc., Perkin Trans. 1 (1990), (1), 123-8

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:114913

GΙ

AB 1,3-Disubstituted 5-cyanouracils react with thioureas and guanidines to give the 5-carbamoyl-2-thiocytosines I (R = H, Me, Bu, Ph; R1 = Me, cyclohexyl) and 2,4-diamino-5-carbamoylpyrimidines II (R = Ph, Me; R1 = Me, H), resp. On the other hand, 1-aryl-5-cyanouracils react with thioureas to give 7-aminopyrimido [4,5-d]pyrimidine-2,4-diones III (R =

H, Me; R2 H, OMe).

IT 94839-44-8P 101989-67-7P 128836-42-0P 129088-65-9P

RN 94839-44-8 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-amino-1,3-dimethyl- (9CI) (CA INDEX NAME)

RN 101989-67-7 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-amino-3-methyl-1-phenyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} & \\ & \\ H_2N & N & N \\ N & N & N \\ & N & Me \\ \end{array}$$

RN 128836-42-0 CAPLUS
CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione,
7-amino-1-(4-methoxyphenyl)-3methyl- (9CI) (CA INDEX NAME)

RN 129088-65-9 CAPLUS
CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 3-methyl-7-(methylamino)-1-phenyl- (9CI) (CA INDEX NAME)

L4 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2000 ACS ACCESSION NUMBER: 1987:162576 CAPLUS

DOCUMENT NUMBER: 106:162576

TITLE: Preparation and formulations of pyrimido[4,5-

d]pyrimidine derivatives as antiallergics

INVENTOR(S): Kitamura, Norihiko; Onishi, Akimoto

PATENT ASSIGNEE(S): Nippon Zoki Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent Japanese

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| | | | | |
| JP 61249988 | A2 | 19861107 | JP 1985-90357 | 19850425 |
| JP 06013518 | B4 | 19940223 | | |

GI

The title compds. (I; R1, R2 = alkyl; R3 = NH2, alkylamino; R4 = H, AB alkyl,

Ph, NH2) are prepd. from uracil derivs. (I; R1 and R2 = alkyl; Y = NH2, halo, dialkylaminomethyleneamino) and H2NZ (Z = C:XR4; X = O, NH; R4 = H, alkyl, Ph, NH2). Thus, 6-amino-5-cyano-1,3-dimethyluracil was cyclized with formamide to give 5-amino-1, 3-dimethylpyrimido[4,5-d]pyrimidine-2, 4dione (III). III at 100 mg/kg in rats inhibited allergic reactions. A tablet contained III 10, lactose 130, starch 40, and Mg stearate 10 mg.

56007-62-6P ΙT

RL: PREP (Preparation)

(prepn. of, as antiallergic)

RN 56007-62-6 CAPLUS

Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 5,7-diamino-1,3-dimethyl-CN (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \\ \\ \text{H}_2\text{N} & \text{N} & \text{N} \\ \\ & \text{N} & \text{N} & \text{N} \\ \\ & \text{NH}_2 & \text{O} \end{array}$$

ANSWER 7 OF 10 CAPLUS COPYRIGHT 2000 ACS 1986:186439 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER:

104:186439

TITLE:

Pyrimidopyrimidinedione derivatives and their use as

anti-allergic agents

09/ 422,451

INVENTOR(S):

Kitamura, Norihiko; Ohnishi, Akimoto

PATENT ASSIGNEE(S):

Nippon Zoki Pharmaceutical Co., Ltd., Japan

SOURCE:

Eur. Pat. Appl., 51 pp.
CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------------------|--------------|---------------------------|----------------------------------|----------------------|
| EP 163599
EP 163599 | A2
A3 | 19851204
19870225 | EP 1985-810182 | 19850424 |
| EP 163599 | В1 | 19900321 | | |
| R: AT, BE,
JP 60226882 | CH, DE
A2 | , FR, GB, IT,
19851112 | LI, LU, NL, SE
JP 1984-83557 | 19840424 |
| JP 05059118 | В4 | 19930830 | N. 1005 010100 | 10050404 |
| AT 51231
US 4886807 | E
A | 19900415
19891212 | AT 1985-810182
US 1988-277447 | 19850424
19881129 |
| PRIORITY APPLN. INFO | .: | | JP 1984-83557
EP 1985-810182 | 19840424
19850424 |
| | | | US 1985-726618 | 19850424 |

GI

AB The title compds. (I; R1 = alkyl; R2 = alkyl, Ph; R3 = H, alkyl, alkylamino; R4 = H, (halo)alkyl, Ph, amino, alkylamino) were prepd. Thus,

6-amino-1,3-dimethyluracil underwent Vilsmeier reaction with HCONMe2 to give 95% 5-[(dimethylamino)methylene]-5,6-dihydro-6-imino-1,3-dimethyluracil which was refluxed with thiourea in EtOH contg. NaOEt to give 52% I (R1 = R2 = Me, R3 = H, R4 = NH2) (II). In rats 20 mg II/kg orally gave 53.3% inhibition of passive cutaneous anaphylaxis reaction compared to 67.3% for theophylline.

IT 56007-62-6P 94839-44-8P 94839-45-9P 101989-67-7P 101989-73-5P 101989-74-6P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of, as allergy inhibitor)

RN 56007-62-6 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 5,7-diamino-1,3-dimethyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \\ \\ \text{H}_2\text{N} & \text{N} & \text{N} \\ \\ & \text{N} & \text{N} & \text{N} \\ \\ & \text{NH}_2 & \text{O} \end{array}$$

RN 94839-44-8 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-amino-1,3-dimethyl- (9CI) (CA INDEX NAME)

RN 94839-45-9 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 1,3-dimethyl-7-(methylamino)-(9CI) (CA INDEX NAME)

RN 101989-67-7 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-amino-3-methyl-1-phenyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} \\ & \\ \text{H}_2\text{N} & \text{N} & \text{N} \\ & & \\ \text{N} & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

RN 101989-73-5 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-amino-1,3-diethyl- (9CI) (CA INDEX NAME)

RN 101989-74-6 CAPLUS

Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-amino-3-methyl-1-(2-CN methylpropyl) - (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} i-Bu \\ \downarrow \\ H_2N \\ N \\ N \\ N \\ Me \\ O \end{array}$$

ANSWER 8 OF 10 CAPLUS COPYRIGHT 2000 ACS L4

ACCESSION NUMBER: 1985:95601 CAPLUS

DOCUMENT NUMBER: 102:95601

TITLE: A facile synthesis of 7-substituted

pyrimido[4,5-d]pyrimidine-2,4-diones

Hirota, Kosaku; Kitade, Yukio; Sajiki, Hironao; Maki, AUTHOR(S):

Yoshifumi

CORPORATE SOURCE: Gifu Pharm. Univ., Gifu, 502, Japan

SOURCE: Synthesis (1984), (7), 589-90

CODEN: SYNTBF; ISSN: 0039-7881

Journal DOCUMENT TYPE:

English LANGUAGE:

GΙ

09/ 422,451

AB Cyclization of uracil I with RC(X)NH2 (R = H, Me, CF3, Ph, H2N, MeNH; X = 0, S, NH) gave 52-92% 7 title compds. II.

IT 94839-44-8P 94839-45-9P

RN 94839-44-8 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 7-amino-1,3-dimethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \\ \\ \text{H}_2\text{N} & \text{N} & \text{N} \\ & \\ \text{N} & \text{Me} \\ & \\ \text{O} & \\ \end{array}$$

RN 94839-45-9 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 1,3-dimethyl-7-(methylamino)-(9CI) (CA INDEX NAME)

L4 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER:

1981:156846 CAPLUS

DOCUMENT NUMBER:

94:156846

TITLE:

Phosgeniminium salts. Part 28. Annelation of 5 or 6

membered heterocycles to uracil derivatives via

phosgeniminium salt condensation

AUTHOR (S):

Kokel, B.; Lespagnol, C.; Viehe, H. G.

CORPORATE SOURCE:

Lab. Chim. Org., Univ. Louvain, Louvain-la-Neuve,

B-1348, Belg.

SOURCE:

Bull. Soc. Chim. Belg. (1980), 89(8), 651-7

CODEN: BSCBAG; ISSN: 0037-9646

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI

AB Reaction of the uracil I (R = NH2, R1 = H) with Me2N+:CCl2Cl- gave I (R = NH2, R1 = CCl:N+Me2Cl-) which reacted with nucleophiles to give I [R = NH2, R1 = CXNMe2, X = O, NPh, NNH2, NCN, C(CN)2]. The latter 2 compds. were hydrolyzed to II (X1 = N, CCN). Reaction of, I (R = OH, R1 = H)

with

Me2N+:CCl2Cl- gave III which also reacted with nucleophiles to give I (R

OH, R1 = CXNMe2, X = NH, NPh, NOH). The latter compd. was cyclized by heating to IV.

IT 77008-19-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 77008-19-6 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione,

7-amino-5-(dimethylamino)-1,3-

dimethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & \text{Me} \\ & & \\ & & \\ & & \\ \text{Me}_{2} \text{N} & \text{O} \\ & &$$

L4 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1976:74208 CAPLUS

DOCUMENT NUMBER: 84:74208

TITLE: Cycloacylation of enamines. III. Synthesis and

reactions of pyrimido[4,5-d]pyrimidines

AUTHOR(S): Grohe, Klaus; Heitzer, Helmut

CORPORATE SOURCE: Zent. Forsch., Bayer A.-G., Leverkusen, Ger.

SOURCE: Justus Liebigs Ann. Chem. (1975), Volume Date 1974,

(12), 2066-73 CODEN: JLACBF

09/ 422,451

DOCUMENT TYPE: Journal LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB Reaction of the 4-aminouracils I with C13CN:CC12, C13CCC1:NCC12CC13, PhCC12N:CC12, or C13CCC12NCO gave by cycloacylation the pyrimidopyrimidines II (R = Me, CH2CH2Ph, CH2:CHCH2, or H; R1 = Me, R2 = CC13, R3 = C1), II (R = R1 = Me, R2 = C1, R3 = Ph) and II (R = R1 = Me,

R2 = Ph, R3 = Cl), or II (R = R1 = Me, R2 = CCl3, R3 = OH), resp. Some nucleophilic substitution reactions of III were reported.

IT 56007-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and reaction with nitrofuraldehyde)

RN 56007-74-0 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4,7(1H,3H,6H)-trione, 5-(ethylamino)-1,3-dimethyl-, 7-hydrazone (9CI) (CA INDEX NAME)

IT 56007-61-5P 56007-62-6P 56007-63-7P 56007-64-8P 56007-65-9P 56007-66-0P 56007-71-7P 56007-75-1P

RN 56007-61-5 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 5,7-bis(ethylamino)-1,3-dimethyl- (9CI) (CA INDEX NAME)

RN 56007-62-6 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 5,7-diamino-1,3-dimethyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \\ \\ H_2N \\ N \\ N \\ N \\ NH_2 \\ O \\ \end{array}$$

RN 56007-63-7 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 1,3-dimethyl-5,7-bis[(1-methylethyl)amino]- (9CI) (CA INDEX NAME)

RN 56007-64-8 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 5,7-bis(butylamino)-1,3-dimethyl- (9CI) (CA INDEX NAME)

RN 56007-65-9 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 5,7-bis(dodecylamino)-1,3-dimethyl- (9CI) (CA INDEX NAME)

RN 56007-66-0 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 1,3-dimethyl-5,7-bis[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 56007-71-7 CAPLUS

CN Pyrimido[4,5-d]pyrimidine-2,4(1H,3H)-dione, 5,7-bis(ethylamino)-1,3-di-2-propenyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2-\text{CH} \longrightarrow \text{CH}_2 \\ \\ \text{EtNH} & \text{N} & \text{O} \\ \\ \text{N} & \text{N} & \text{CH}_2-\text{CH} \longrightarrow \text{CH}_2 \\ \\ \text{EtNH} & \text{O} \end{array}$$

RN 56007-75-1 CAPLUS

CN 2-Furancarboxaldehyde, 5-nitro-, [4-(ethylamino)-5,6,7,8-tetrahydro-6,8-dimethyl-5,7-dioxopyrimido[4,5-d]pyrimidin-2-yl]hydrazone (9CI) (CA INDEX

NAME)

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(FILE 'HOME' ENTERED AT 09:11:18 ON 09 FEB 2000)

FILE 'REGISTRY' ENTERED AT 09:11:26 ON 09 FEB 2000 STRUCTURE UPLOADED

L2 2 S L1 L3 72 S L1 FUL

FILE 'CAPLUS' ENTERED AT 09:12:09 ON 09 FEB 2000

L4 10 S L3

=> log y

COST IN U.S. DOLLARS
SINCE FILE TOTAL
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FULL ESTIMATED COST
40.22
166.67

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL
ENTRY SESSION
CA SUBSCRIBER PRICE

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-5.57

STN INTERNATIONAL LOGOFF AT 09:13:24 ON 09 FEB 2000